

## Ligand-breeding procedure

FIG. 1

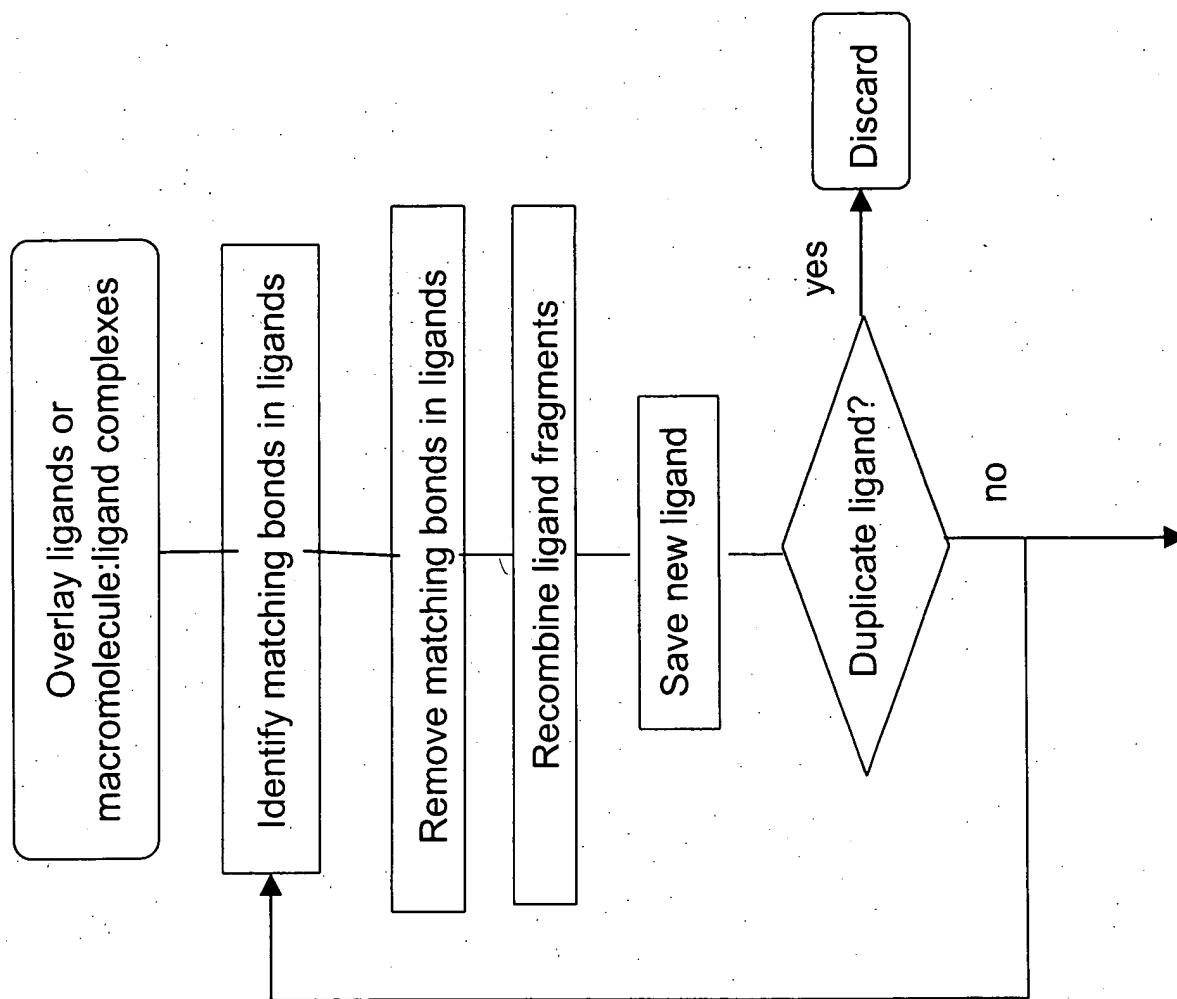
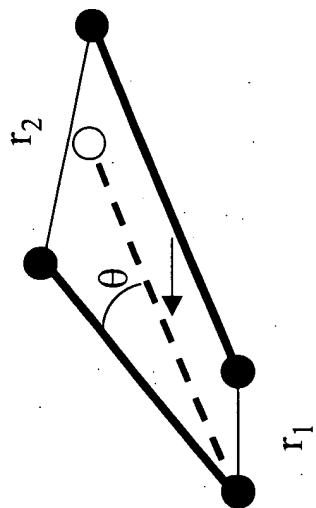
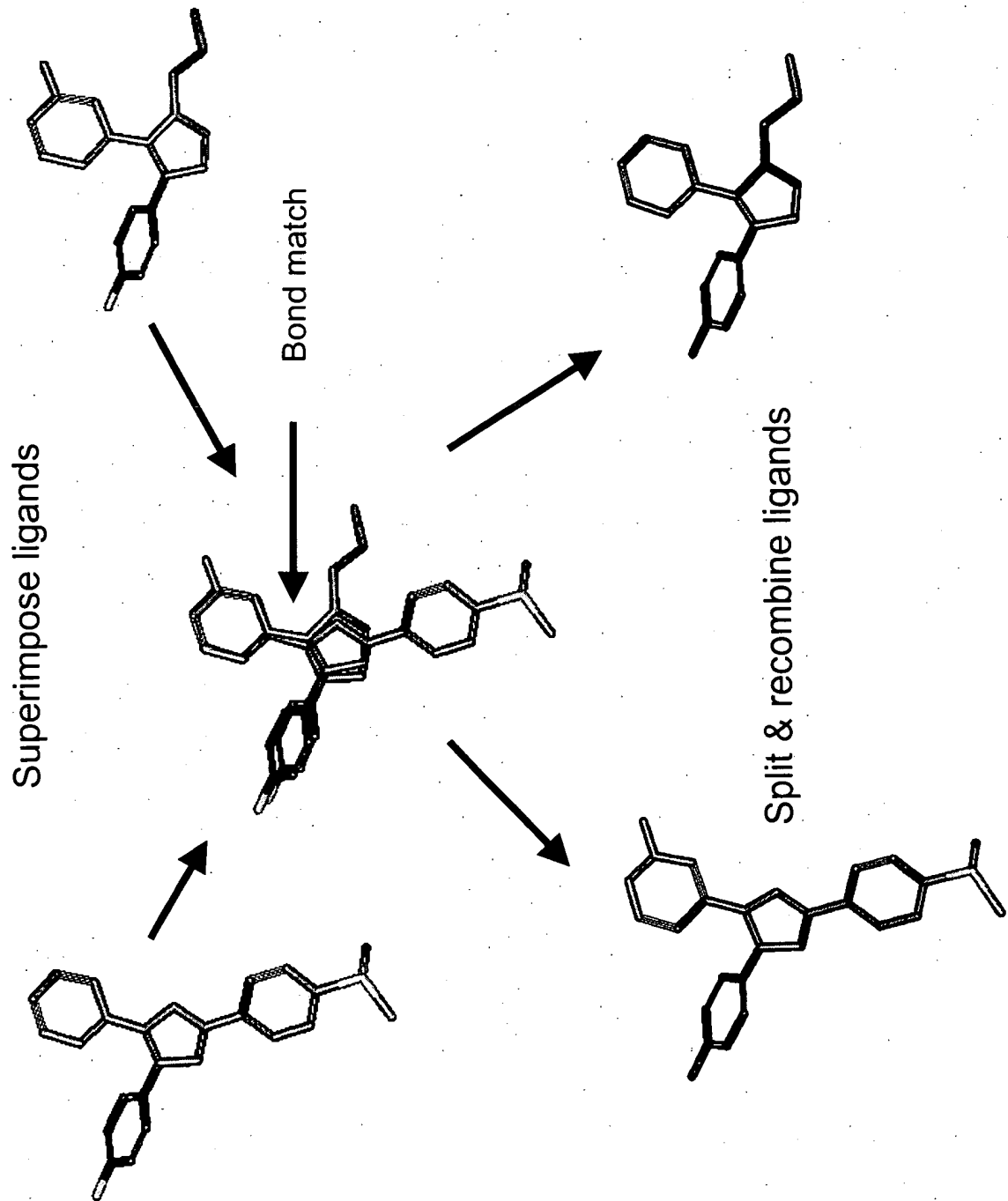


FIG. 2

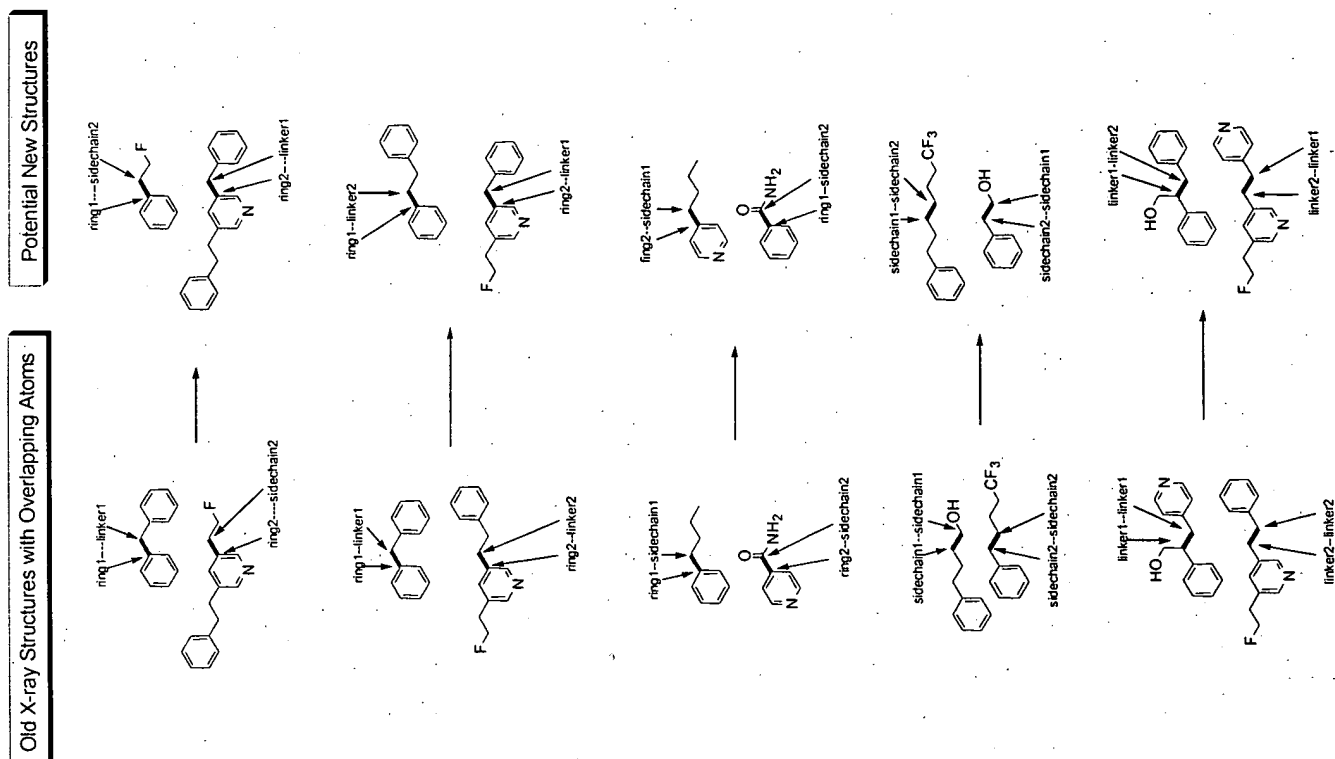


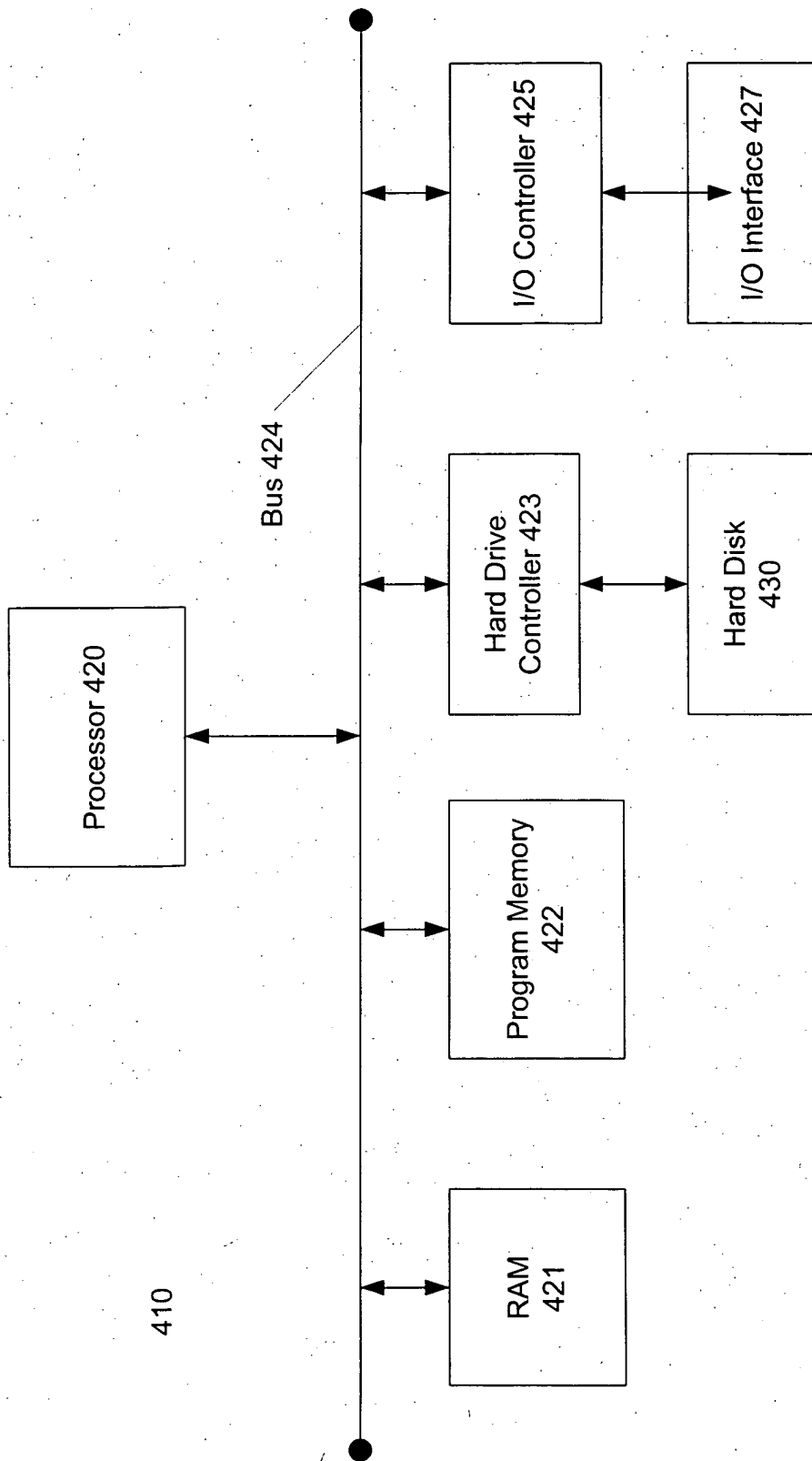
Dark circles represent atoms, thick lines represent bonds. Thin lines show  $r_1$  and  $r_2$ , the distances between the atoms at each end of the bond. The dashed line shows the right-hand bond translated left so that the angle between the two bonds,  $\theta$ , can be calculated.

FIG.3



**FIG. 4**





**FIG. 5**

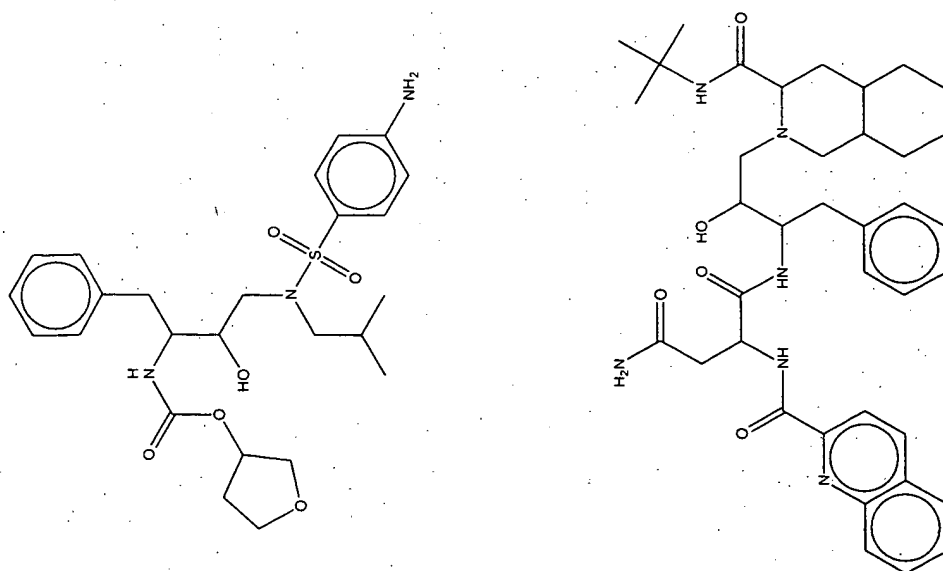
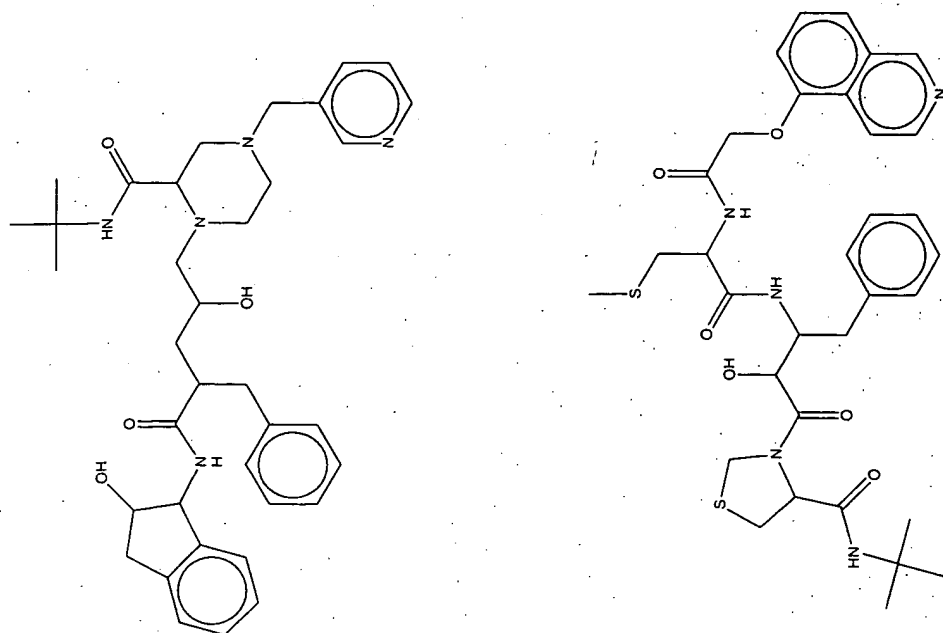


FIG. 6

FIG. 7

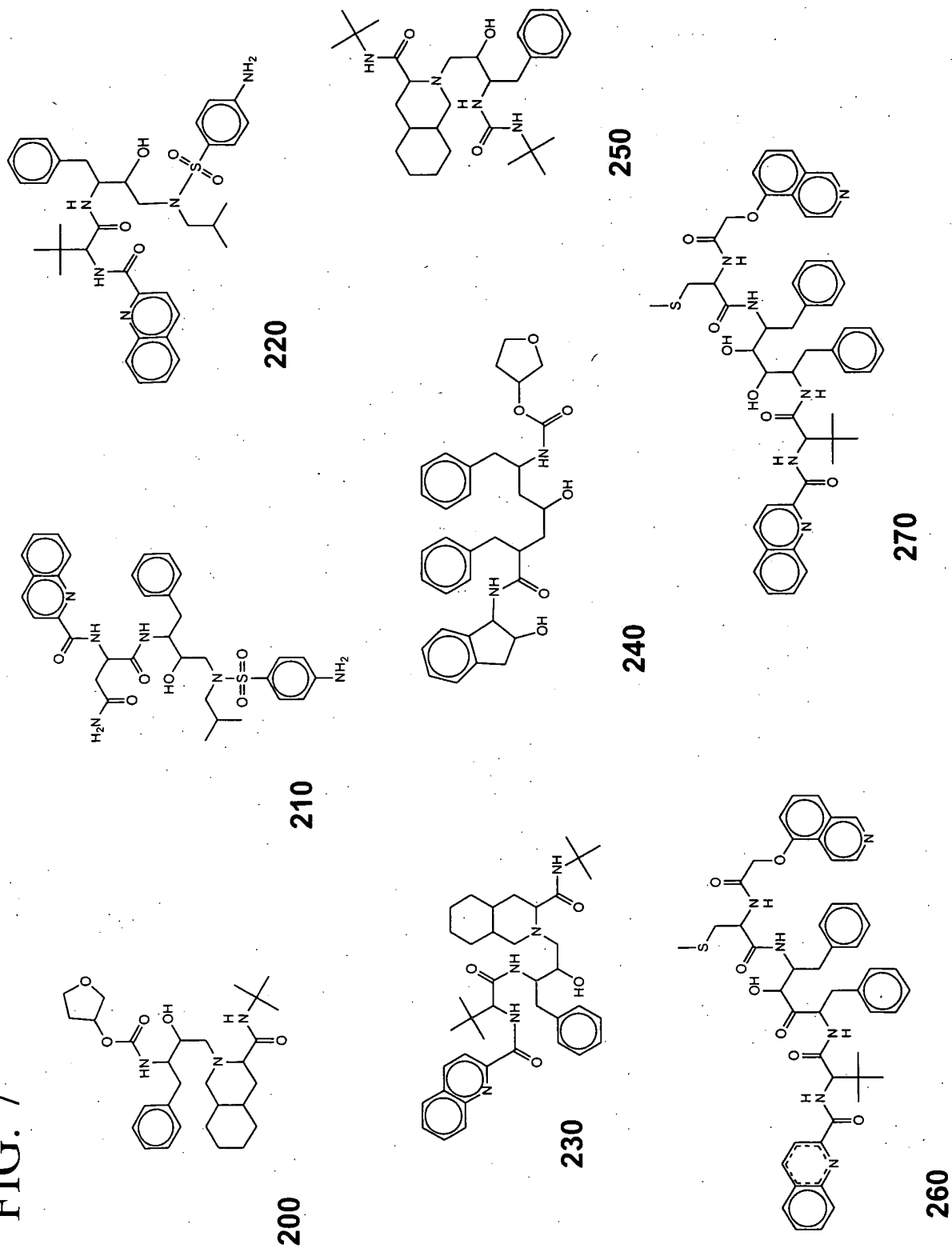
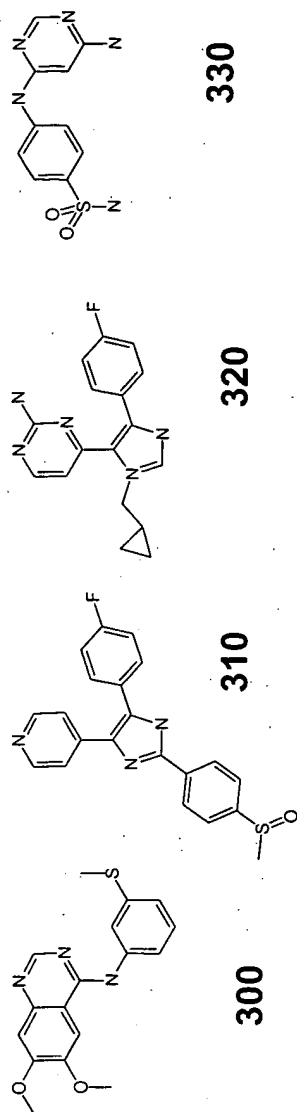


FIG. 8

Starting ligands



Output ligands

